P8073 US

Reflector for X-Ray Radiation

This application claims Paris Convention priority of DE 102 54 026.8 filed November 20, 2002 the complete disclosure of which is hereby incorporated by reference.

BACKGROUND OF THE INVENTION

The invention concerns a reflector for X-ray radiation which is curved in a non-circular arc shape along a first cross-section in a plane containing an x-direction (tangential curvature), wherein the reflector is also curved along a second cross-section in a plane perpendicular to the x-direction (sagittal curvature).

An X-ray mirror of this type is disclosed e.g. in DE 44 07 278 A1.

X-ray radiation is electromagnetic radiation as is visible light. Due to the higher energy on the order of keV, the interaction between X-ray radiation and matter is significantly different than with visible light. Considerable difficulties were found in providing effective optical structural elements such as mirrors or lenses for X-ray radiation. The structural elements realized up to now are based mainly on Bragg diffraction and total reflection, both under grazing incidence.

In a flat embodiment, an X-ray mirror on the basis of the Bragg diffraction can only reflect a very small portion of the incident

divergent X-ray radiation, since the Bragg condition requires relatively accurate angles of incidence. To solve this problem, curved mirror surfaces and also a locally variable planar separation were suggested. The curvature of the mirror surface and the planar separation may thereby vary along a first direction x which corresponds approximately to the main propagation direction of the X-ray radiation (under grazing incidence). For normal dimensions of X-ray analysis devices, the local radius of curvature is on the order of meters and usually has a parabolic or elliptical shape. It is technically relatively easy to produce. To realize a variable planar separation, a multi-layer mirror design has been used. This type of X-ray mirror is referred to as a "Goebel Mirror" (DE 44 07 278 A1).

The reflectivity of the Goebel mirror is limited in that the divergence of the beam perpendicular to the x-direction in the mirror plane cannot be satisfactorily taken into consideration. Two-dimensional focusing is feasible through a rotationally symmetrical design i.e. a second circular arc-shaped mirror curvature in the plane perpendicular to the x-direction. For typical dimensions of X-ray analysis devices, the mirror must have radii of curvature perpendicular to the x-direction in the millimeter range. It has not been previously possible to produce such a strongly curved X-ray mirror with sufficient accuracy, since sufficiently precise reduction in the surface roughness and waviness of such a strongly curved mirror is difficult. Moreover, it has not been possible up to now to prevent layer thickness errors for multi-layer mirrors in the region of large radii of curvature (i.e. at the mirror edge) using conventional coating techniques (sputtering, molecular beam epitaxy etc.), with a reasonable degree of effort. These coating errors reduce the

reflectivity of the X-ray mirrors for the desired X-ray wavelength and introduce scattered rays of other wavelengths.

To still obtain two-dimensional focusing, two one-dimensionally focusing Goebel mirrors, which are rotated relative to each other through approximately 90°, must be used in series. This causes considerable intensity loss.

Another disadvantage of rotationally symmetrical Goebel mirrors is the circular annular beam profile of the reflected X-ray radiation outside of the focus. Either the sample or the detector is usually in the focus and therefore either the detector or the sample must be disposed in the region of the annular beam profile. This reduces the intensity, and the optical path of such an X-ray analysis device lacks flexibility due to the annular beam profile.

Rotationally symmetrical total reflection mirrors with two-dimensional focusing are also known. Due to the reduced light collecting capacity, the very small maximum angle of incidence, the associated adjustment difficulties, and the lack of monochromatization, total reflection mirrors are no practical alternative.

In contrast thereto, it is the object of the present invention to make the design of X-ray mirrors and the beam shape of reflected X-ray radiation more flexible, to facilitate production of X-ray mirrors with high efficiency (i.e. high reflection capacity and good focusing properties).

SUMMARY OF THE INVENTION

This object is achieved in a surprisingly simple but effective fashion by a reflector for X-ray radiation (X-ray mirror) of the above-presented type which is characterized in that the reflector has a curvature along the second cross-section which is also not circular arc-shaped.

The curvature along the second cross-section (sagittal curvature) is particularly critical for the production of two-dimensional focusing mirrors. In accordance with the invention, this second curvature is not circular arc-shaped. In particular, deviations, which reduce the curvature of the reflector along the second cross-section and in particular in the edge region of the reflector, are of particular importance. The polishing processes for reducing the roughness or waviness of the reflector surface can be greatly facilitated.

A deviation from the rotationally symmetrical shape also offers new design possibilities for the beam shape of the reflected X-rays outside of the focus. The circular annular shape outside of the focus can be eliminated and appropriate design of the curvature of the inventive reflector along the second cross-section can be used to adjust the beam shape to the requirements of a particular experiment. Possible alternative beam shapes include an elliptical, annular shape and a lens-type shape. The beam shape can, in particular, be adjusted to the shape of a sample to be examined, to an X-ray detector, or an entrance slit thereof.

The deviation from the curvature along the second cross-section also permits compensation of coating errors in multi-layer mirrors, without reducing the reflectivity of the X-ray mirror (see below).

In an advantageous embodiment of the inventive reflector, the curvature of the reflector along the second cross-section adjusts the focusing properties of the reflector, in particular in the plane perpendicular to the x-direction. The curvature of the reflector along the second cross-section determines the direction of the outgoing X-rays, which, upon incidence initially diverge in the reflector plane perpendicular to the x-direction. The focusing effect of the curvature along the second cross-section can preferably be selected such that the focus of both curvatures of the reflector coincide e.g. at the detector or at infinity (parallel beam).

One embodiment of the inventive reflector is particularly advantageous wherein the reflector focuses or renders parallel in two dimensions. This produces a high intensity of the outgoing X-rays since only one loss-causing reflection on the inventive reflector is required for two-dimensional focusing or parallelization of the X-rays.

In a further advantageous embodiment, the reflector is curved parabolically, hyperbolically or elliptically along the first cross-section (tangential curvature). The parabolic shape is the basic shape of the Goebel mirror and permits parallelization of the outgoing X-rays, which exhibit a beam divergence when incident on the reflector across the mirror surface in the x-direction. An elliptical shape permits focusing of the initially divergent beam to a specific focal spot.

The preferred embodiment of the inventive reflector is characterized in that the reflector has a periodically repeating sequence of layers of materials A, B, ... with different refractive indices, wherein the sum $d = d_A + d_B + \dots$ of the thicknesses d_A, d_B, ... of sequential layers of

materials A, B, ... changes continuously along the x-direction, in particular, monotonically. This embodiment corresponds to a Goebel mirror whose curvature along the second cross-section is not circular arc-shaped. Up to now it has not been technically possible to produce Goebel mirrors with rotationally symmetrical second curvature of satisfactory quality. The above-mentioned embodiment is far easier to produce than a rotationally symmetrical Goebel mirror and has comparable X-ray optical properties. The change in the angle of incidence on the multi-layer across the length of the X-ray mirror from the front to the back (in the x-direction) is compensated for with respect to the Bragg condition through adjusting the layer separation (planar separation) to ensure good reflectivity for the X-ray radiation of a given wavelength over the entire length of the X-ray mirror. Focusing of the beam divergence perpendicular to the x-direction in the mirror plane is adjusted via the non-circular arc shaped curvature along the second cross-section, a shape which generally produces incomplete focusing. This may be desired for certain applications and is therefore explicitly part of the present invention.

A further particularly advantageous development of this embodiment is characterized in that the sum d changes along the second cross-section, in particular by more than 2%. The change in the sum d along the second cross-section is an almost unavoidable error when coating strongly curved surfaces. The curvature is particularly strong in the edge region of the reflector and for this reason, in conventional coating methods, the layer thickness there is smaller than at non-curved, flat locations. When the layer thickness changes, the angle of incidence of the radiation must be adjusted to ensure further fulfillment of the Bragg equation and thereby ensure sufficient reflectivity for a given wavelength. The angle of incidence is a

function of the local curvature of the reflector. When the curvature dependence of the coating thickness is known (e.g. by model calculation described below, or experimentally) the actual reflection and focusing behavior of the finished multi-layer reflector can be determined and adjusted through precise previous setting of the curvature of the mirror.

In one particularly advantageous embodiment of this further development, the curvature of the reflector along the second cross-section effects focusing and reflectivity properties of a reflector having changes in the sum d along the second cross-section which correspond to those of a reflector having circular curvature along its second cross-section and a constant sum d. This design realizes an X-ray optical component whose properties correspond to a rotationally symmetrical Goebel mirror. Realization of a functioning rotationally symmetrical Goebel mirror has not been possible up to now. Production of this inventive embodiment is easier since the curvature along the second cross-section is reduced and the unavoidable layer thickness errors can be accepted.

In another advantageous embodiment, the reflector has an elliptical curvature with different semi-axis lengths or a parabolic curvature along the second cross-section. The elliptical structure is particularly suited for focusing the divergence of radiation perpendicular to the x-axis in the mirror plane. The parabolic shape promotes formation of a parallel beam.

In an advantageous embodiment of the inventive reflector, the reflector has a reflecting surface of a width of more than 2mm, in particular at least 4mm (measured perpendicular to the x direction).

In conventional rotationally symmetrical Goebel mirrors, the reflectivity decreases towards the edge for a given wavelength. In particular, for conventional dimensions of an X-ray analysis device, reflecting widths are limited to less than 2mm. The inventive reflector has a high reflectivity for much larger widths. This increases the reflected intensity in accordance with the invention, to first approximation, in proportion to the reflecting surface.

The present invention also concerns an X-ray analysis device with an X-ray source, a sample to be analyzed, an X-ray detector, beam-forming and/or beam-delimiting means and the inventive reflector described above. The inventive reflector is particularly advantageous when used in such an X-ray analysis device. In addition to an X-ray tube, the X-ray source may comprise a separate monochromator. The sample may be disposed on a goniometer. The detector may be designed to resolve energy or be integrally event counting.

In a preferred embodiment of the inventive X-ray analysis device, the X-ray radiation impinges on the reflector at an angle of less than 5° with respect to the x-direction. Bragg diffraction is particularly effective under these circumstances, since, for conventional X-ray radiation in the region of some keV (e.g. Cu-Kα), the associated layer thickness is technically easy to realize.

In another advantageous embodiment, the curvature of the reflector along the second cross-section is designed such that the reflectivity of the reflector is maximum for the wavelength of the radiation generated by the X-ray source. This leads to high reflecting intensities and therefore shorter measuring times in the X-ray analysis device.

In particular, different reflectors may be exchanged for use with different X-ray wavelengths.

One embodiment is particularly advantageous wherein the reflector focuses X-ray radiation incident thereon to a point-like region (focal spot), in particular onto the sample or the X-ray detector. These are the most frequent applications for an optical path, since the counting rate on the detector is thereby maximized.

One embodiment of an inventive X-ray analysis device is also advantageous with which the reflector generates an X-ray beam from the incident X-ray radiation having a desired beam divergence, in particular a parallel beam. Parallel beams can illuminate samples with high uniformity and a similar beam profile can be projected on both the sample and the detector.

Further advantages of the invention can be extracted from the description and the drawing. The features mentioned above and below can be used in accordance with the invention either individually or collectively in arbitrary combination. The embodiments shown and described are not to be understood as exhaustive enumeration, rather have exemplary character for describing the invention.

The invention is shown in the drawing and is explained in more detail with reference to embodiments.

BRIEF DESCRIPTION OF THE DRAWING

Fig. 1a shows an inventive X-ray analysis device with schematic representation of a beam divergence, which sweeps over an inventive reflector in the x-direction;

Fig. 1b shows the X-ray analysis device of Fig. 1a with schematic representation of a beam divergence, which sweeps over the reflector in the mirror plane perpendicular to the x-direction;

Fig. 2a shows the inventive reflector of Fig. 1a and a first cross-section in a plane, which contains the x-direction;

Fig. 2b shows the inventive reflector of Fig. 1a and a second cross-section in a plane perpendicular to the x-direction;

Fig. 3 shows a cross-section through a rotationally symmetrical reflector (prior art);

Fig. 4 shows a cross-section through an inventive, non-rotationally symmetrical reflector;

Fig. 5 shows the construction of a monocrystal diffractometer for protein crystallography according to prior art;

Fig. 6 shows the beam image of a rotationally symmetrical, focusing reflector in the image focus and outside of the image focus (prior art);

Fig. 7 shows the beam image of a segment of a two-dimensional focusing reflector in the image focus and in front of the image focus (prior art);

Fig. 8 shows a section of a rotationally ellipsoidal focusing reflector (prior art);

Fig. 9 shows the depth dependence of the reflector of Fig. 8 in the x direction;

Fig. 10 shows the depth dependence of the reflector of Fig. 8 in the y direction;

Fig. 11 shows the local angle of inclination of the reflector surface of the reflector of Fig. 8 along the y-axis at x=90mm;

Fig. 12 shows the structure of a conventional coating device for coating a reflector without prevention of coating errors (prior art);

Fig. 13 shows the behavior of the relative coating thickness (coating error) at the reflector surface of the reflector of Fig. 8 in the y-direction at x=90mm;

Fig. 14a shows the reflectivity over the surface of a rotationally-ellipsoidal reflector with dimensions 60 x 4 mm assuming a cos(β)-coating error for Cu-Kα-radiation;

Fig. 14b shows the reflectivity over the surface of a rotationally ellipsoidal reflector with dimensions 60 x 4 mm assuming a cos(β)-coating error for Cu-Kβ-radiation;

Fig. 15 shows a structure of a coating device for homogeneous coating of a reflector;

Fig. 16 shows the inventive compensation curve of a cos(β)-coating error using a non-rotationally symmetrical ellipsoid.

DESCRIPTION OF THE PREFERRED EMBODIMENT

Fig. 1 schematically shows the structure of an inventive X-ray analysis device. The X-ray source 1 emits X-ray radiation. Fig. 1a shows two beams 2 and 3 of this X-ray radiation. Both beams 2, 3 pass a collimator 4 and are incident on the reflecting surface of the inventive reflector 5. An orthogonal coordinate system X, Y, Z is associated with the reflector 5. The reflector is a gradient multi-layer mirror. The reflecting surface in the z-direction is formed by a periodic sequence of at least two layers of materials A, B with different refractive indices for the incident X-ray radiation. The respective layers extend approximately in neighboring XY planes. The reflecting surface of the reflector 5 is curved in two dimensions (see Fig. 2a and 2b). In accordance with the invention, neither of the two curvatures has the shape of a circular arc.

The beams 2, 3 are reflected on the reflector 5, penetrate through the sample 6 and are registered in the X-ray detector 7.

The beams 2, 3 have a divergence 8 in the XZ plane of typically 0.2 to 2°. The angle of incidence 9 of the two beams 2, 3 is thereby approximately 0.5 to 2.5° with respect to the X direction or the X' direction (the angle of incidence 9 is exaggerated in Fig. 1a and also in Fig. 1b for reasons of clarity). The X-direction is the main direction of extension of the reflector 5. Apart from the angle of incidence 9, the direction of incidence of the X-ray radiation on the reflector 5 coincides with the X-direction.

The divergence 8 of impinging X-ray radiation in the XZ plane is focused through the curvature of the reflector along its first cross-section (tangential curvature) in the XZ plane, i.e. the plane containing the x-direction (see Fig. 2a). In Fig. 1a, the curvature of the reflector along the first cross-section is parabolic.

Fig. 1b shows the same X-ray analysis device as Fig. 1a, however, comprising two other beams 10 and 11. Both beams have a divergence 12 in the YZ plane. The order of magnitude of this divergence 12 is approximately 1-2°. The beams 10, 11 are reflected at the surface of the reflector 5, penetrate through the sample 6 and are registered in the detector 7.

The divergence 12 of the incident X-ray radiation in the YZ plane is focused by the curvature of the reflector along a second cross-section (sagittal curvature) in the YZ plane, i.e. perpendicular to the x-direction (see Fig. 2b). In contrast to the conventional Goebel mirror, the inventive reflector 5 has a curvature, which is not circular arc shaped, but approximately elliptical.

The curvature of the reflector 5 is shown in Figs. 2a and 2b. Both figures show the reflector 5 of Fig. 1a/b in an enlarged scale. The intersection line 13 of the reflecting surface of the reflector 5 and XZ plane (which contains the X direction) illustrates the curvature of the reflector in a first dimension. In Fig. 2a, this curvature is parabolic. The first curvature represents the curvature of the reflector along the first cross-section.

The intersection line 14 of the reflecting surface of the reflector 5 in the YZ plane illustrates the curvature of the reflector in a second dimension. In Fig. 2b, this curvature is elliptical. This second curvature represents the curvature of the reflector along the second cross-section and, in accordance with the invention, does not have the shape of a circular arc. In this embodiment, the reflector surface is mirror-symmetrical relative to a central XZ plane. This is generally advantageous for the invention to obtain uniformly illuminating reflected X-rays.

The inventive device is explained in detail below for X-rays incident on two-dimensionally curved X-ray reflectors, in particular multi-layer X-ray reflectors with a shape other than rotationally symmetrical.

X-ray radiation reflectors having a multi-layer structure have been used in different X-ray analysis instruments for some time. These multi-layers typically consist of some ten to some hundred individual alternating layers of two or more materials, with individual layer thickness of typically 1-20nm. These multi-layers deflect and monochromatize incident X-rays through diffraction in correspondence with the Bragg equation. The reflectivity of these multi-layers may be very high for X-rays. Reflectivities of up to 90%

were theoretically predicted and also obtained in experiments through continuous improvements in manufacturing coating techniques. For actual spatially extended X-ray sources (in contrast to theoretical, ideal point sources) the reflectivities are reduced to typically 30-70%, depending on the source size. For use in the region of hard X-ray radiation (wavelengths typically 0.05-0.25nm), the deflection angles are typically in the region between 0.5 – 2.5 degrees: within the range of grazing incidence.

Substantial improvements in such X-ray reflectors were obtained e.g. in US 6,226,349 and in M. Schuster, H. Göbel, L. Brügemann, D. Bahr, F. Burgäzy, C. Michaelsen, M. Störmer, P. Ricardo, R. Dietsch, T. Holz and H. Mai "Laterally graded multi-layer optics for X-ray analysis", Proc. SPIE 3767, pp. 183-198, 1999 by curving the reflectors in one dimension (parabolically, elliptically, etc.). The requirements for the shape accuracy of these reflectors are high and are in a region of considerably less than 1 micrometer. To obtain high reflectivity for such reflectors at all locations of the reflector, the multi-layer coatings must vary in a highly defined manner over the surface of the reflector according to the conditions e.g. disclosed in US 6,226,349 and the above cited Schuster publication. The requirements for precision of the coating of such reflectors are quite high and are typically 1-3% of the individual layer thicknesses. These tolerances result from the widths of the multi-layer Bragg reflections, which are typically in the region of 1-3% of the Bragg angle. This results in tolerance requirements for the coating, which are typically in the region of some tens of picometers. Despite these extreme requirements, such reflectors have been recently produced using different methods and have been commercially available for several years.

Since these reflectors are operated with small angles of incidence, the shape is substantially flat (in the range of some ten micrometers) and the radii of curvature are typically a few meters. Macroscopically seen, the reflectors are substantially flat. Due to the curvature of the reflectors, coating of these macroscopically flat reflectors produces no additional problems compared to flat reflectors and the coating of these reflectors is also substantially flat.

Two-dimensionally curved rotationally symmetrical reflectors (rotational ellipsoid, rotationally paraboloid, etc. or segments of these shapes) also coated with multi-layers have been suggested many times for X-rays, e.g. US 4,525,853, US 4,951,304, US 5,222,113. However, they were never realized. Reasons therefor are the enormous technical problems with coating (tangentially varying according to US 6,226,349 and at the same time extremely homogeneous (1-3%) in a transverse direction in which the optics is now also curved). The principal reason therefor is that these reflectors must be substantially flat in one direction (radii of curvature in the meter range), but strongly curved perpendicular thereto (sagittal) with typical curvature radii of only a few millimeters, since the reflectors are operated at small angles of incidence. In addition to the need for extremely precise coating in the tangential direction (specified in US 6,226,349), the considerable angles of inclination in the transverse direction lead to coating errors, since the reflectors are no longer flat but macroscopically curved. Since the layer thicknesses of typical coating methods change with the angle of inclination with respect to the coating source, the additional requirement that the layer thickness be homogeneous in a transverse direction (in the

range of a few tens of picometers) is an additional technical challenge. The required coating has not been obtained up to now.

For this reason, two-dimensionally collimating or focusing multi-layer X-ray reflectors have been realized up to now only according to US 6,014,423 and US 6,014,099 and earlier studies [M. Montel, *X-ray Microscopy and Microradiography*, Academic Press, New York, pp. 177 – 185, 1957; V. E. Cosslett and W. C. Nixon, *X-Ray Microscopy*, Cambridge, At The University Press, p. 108 ff, 1960; *Encyclopedia of Physics*, ed. S. Flügge, Vol. XXX: *X-Rays*, Springer Berlin, p. 325 ff, 1957; Kirkpatrick-Baez, see e.g. Fig. 1 in US 6,041,099] through combination of two macroscopically substantially flat reflectors, i.e. through double reflection. Since at least two reflectors must be used which must be precisely mutually aligned, the costs and the adjustment effort are substantial. Moreover, the use of two reflectors results in intensity loss. Since even the best multi-layer reflectors lose efficiency, in particular when used with extended X-ray sources (e.g. rotary anodes), an intensity loss of 50% per reflection is relatively normal for increased extension of the sources. However, these reflectors are up to now the only two-dimensionally collimating or focusing multi-layer X-ray reflectors according to prior art.

For these reasons, all conventional two-dimensionally collimating or focusing rotationally symmetrical X-ray reflectors with sagittal curvature radii in the millimeter range are total reflection mirrors (e.g. WO 0138861 or MICROMIRROR TM Bede Scientific). The requirements for the coating are minimal (only one individual layer is required e.g. gold and the layer must only have a sufficient thickness > approximately 30nm: a homogeneous layer thickness is not required) and meet much lower requirements for the micro roughness

of the reflector compared to a multi-layer reflector (for total reflection approximately 1nm, wherein multi-layer mirrors require a roughness of <0.3nm according to US 6,226,349). Total reflectors have several substantial disadvantages over multi-layer reflectors. They require even smaller irradiation angles (approximately three times smaller), have corresponding reduced light collecting capacity, and lack monochromaticity. Such total reflectors have no monochromatizing properties but only suppress high-energy X-rays for which the total reflection angle is exceeded at certain geometries.

For these reasons, it is extremely desirable to provide improved methods and processes for producing two-dimensionally collimating or focusing multi-layer coated X-ray reflectors.

This is achieved in accordance with the invention by using two-dimensionally curved multi-layer coated bodies, which are not rotationally symmetrical. The advantages that result from the omission of the auxiliary condition of rotational symmetry, are not obvious and are therefore described in the following examples.

The change from a rotationally symmetrical to a non-rotationally symmetrical reflector is initially disadvantageous. This is shown in figures 3 and 4 with the example of a focusing reflector. While the cross-section of rotationally symmetrical reflectors 30 (Fig. 3) is circular and all rays 31 are reflected perpendicularly to the tangent, to a point 32, this is not the case with non-rotationally symmetrical reflectors 40 (Fig. 4). Non-rotationally symmetrical reflectors therefore produce a focusing loss. The free selection of the cross-section offers some additional possibilities as explained by way of example below. It is important (as shown through calculations) that

the focusing loss is horizontal (in width) but not vertical (in height). The reason therefor is that the magnification ratio (source size to image size) of such reflectors is nearly independent of the cross-sectional shape of the reflector. This surprising property can finally be traced back to the high eccentricity of the reflectors relevant in this case (see below).

Fig. 5 shows a typical application (a so-called monocrystal diffractometer). The X-ray radiation 52 emanating from an X-ray source 51 (with collimator 200μm) is focused onto the two-dimensional detector 54 by a rotationally symmetrical reflector 53 (e.g. MICROMIRROR). Due to the finite size of the X-ray source (e.g. 0.1 mm diameter), the beam image at the image focus 61 (see Fig. 6) is also typically some 0.1mm. The sample 55 typically has a diameter of 0.5mm and is typically located 10cm in front of the detector 54. The beam shape 62 is annular at this location. The sample 54 is thereby not optimally illuminated. Conversely, disadvantages occur when the sample is placed at the focus, since the scattered radiation is not point-like at the detector. The fundamentally annular beam profile 62 outside of the image focus is generally disadvantageous.

For this reason, it is sufficient or even advantageous to use only a part (only a segment) of the entire reflector for such applications. Fig. 7 shows that the beam image in the focus 71 (detector) and outside of the focus 72 (sample) has approximately the same size for this section of the reflector. Suitable selection of the reflector and size of the reflector section leads to beam dimensions which are appropriate for the application at hand.

An ellipsoidal reflector section 81 corresponding to Fig. 8 is described by way of example below. The shape of the ellipsoid 82 is described by

$$\frac{(x-a)^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}=1$$

$b=c$ produces a rotationally symmetrical ellipsoid with circular cross-section (prior art). $b \neq c$ produces an inventive non-rotationally symmetrical ellipsoid with elliptical cross-section (all cross-sectional shapes are possible in accordance with the invention). Typical values for a, b and c are a = 250 mm, b = 5 mm, and c = 5 mm. This produces a separation between source and image focus of 2a = 500 mm and a maximum diameter of the reflector 2b = 10 mm. As described above, the necessity of the short curvature radius in the y-z plane results from the auxiliary requirements for small angles of incidence.

Figures 9 and 10 show the corresponding depth profiles along x and y for a 4mm wide reflector section. The curves are substantially flat in the x direction (Fig. 9) and have a drop depth (in the z direction) of some ten micrometers over a length of some ten millimeters, i.e. have a large radius of curvature of typically several meters. The curves along y in accordance with Fig. 10 are macroscopically curved and have a drop depth of several hundred micrometers over a width of 4mm, i.e. have a small radius of curvature in the range of several millimeters. Fig. 11 shows that this strong curvature in the y-z plane produces considerable inclination of the edge of the reflector relative to the horizontal. At the edge of the 4mm wide reflector, angles of inclination β of approximately 30 degrees occur. This edge inclination

produces considerable problems for coating, which must be homogeneous in the y-z plane for a rotationally symmetrical body (in addition to the already mentioned layer thickness gradient along x according to prior art and the extremely high precision required and described therein). The coating methods used for producing X-ray reflectors such as "sputtering" according to US 6,226,349 generally use coating sources with a more or less directed material beam. This has the consequence that, when inclined or tilted surfaces are coated, less material condenses per unit surface than with frontal coating, in dependence on the angle of inclination β (see Fig. 12 with coating source 120, material ray 121, mirror substrate 122 and angle of inclination β). Sputtering produces e.g. approximately a layer thickness distribution which varies with $\cos(\beta)$ wherein β is defined according to $\beta = \arctan(dz/dy)$ (more generally, a dependence with $(\cos\beta)^n$ is observed, wherein n depends on the details of the coating process used. The following is based on a process with n = 1, without limiting the general case). Fig. 13 shows that with such a coating error, the reflector meets the above-mentioned acceptable layer thickness errors of <2% only over a width of less than 2mm.

As shown in Fig. 14, detailed examinations with the Monte-Carlo method (ray tracing) confirm this result (reflectivity for two wavelengths, Cu-Kα and Cu-Kβ, over the surface of a reflector of 60 x 4 mm^2 assuming a cos(β) coating error; light points indicate high reflectivity). These studies also show that the reflector no longer reflects the desired X-ray wavelength in the edge regions (e.g. Cu Kα, Fig. 14a), but also starts to reflect another wavelength in these edge regions due to the decreasing layer thicknesses (e.g. Cu Kβ, Fig. 14b). The reflector loses intensity and also its monochromatic effect.

For coating such a reflector, additional apparative measures to homogenize the layer along the strongly curved surface are required. Fig. 15 (coating source 151, material flow 152) shows two possibilities to homogenize the layer. Movement of a diaphragm 153 or suitable pivoting, reciprocating or other turning motions of the mirror substrate 154 or a combination of these measures can lead to a layer which is homogeneous along the strongly curved surface. It is still necessary to keep to the required layer thickness gradient along the x-direction in a likewise extremely precise fashion as described above. Meeting of this condition in the conventional substantially flat reflectors requires considerable effort with regard to the apparatus (see e.g. DE 19701419) since they generally require, in addition to at least one rotary motion or diaphragm shift, measures to stabilize the temperature or other relevant parameters without impairing the substantially high quality of the vacuum. Controlled coating of strongly curved surfaces additionally requires at least one further rotary motion or diaphragm motion, as described above. The additional apparative effort to meet all these requirements for precision coating in the region of some ten picometers over a three-dimensionally curved surface is extremely high and has not been realized up to now.

The inventive solution does not require any modification of the conventional coating apparatus. Coating systems as used e.g. in Fig. 12 of US 6,226,349 for producing X-ray reflectors can also be used without modification for producing the inventive reflectors. Corresponding to the inventive solution, the semi-axis b is selected such that the above-described coating errors are perfectly

compensated for in case of non-normal incidence. This is described in more detail below.

The rotational ellipsoid is preferably expressed in cylindrical coordinates:

$$\frac{(x-a)^2}{a^2}+\frac{r^2}{b^2}=1$$

wherein $z=r\cdot\cos\alpha$ and $y=r\cdot\sin\alpha$.

To ensure optimum reflection of a rotationally ellipsoidal mirror, the coating thickness *d* must be:

$$d(\alpha)=const.$$

When a coating error occurs, it can be corrected through variation of *b* with α. The rotational ellipsoid becomes the general non-rotationally symmetrical ellipsoid

$$\frac{(x-a)^2}{a^2}+\frac{r^2}{b^2(\alpha)}=1.$$

$b(\alpha)$ is calculated from

$$d(f,\alpha)=\frac{\lambda\cdot b(\alpha)\cdot\sqrt{f\cdot f'}}{2\cdot\left(b^2(\alpha)-\delta\cdot f\cdot f'\right)}$$

[publication Schuster see above]. One obtains

$$b(\alpha)=\frac{1}{2}\cdot\left(\frac{\lambda\cdot\sqrt{f\cdot f'}}{d(f,\alpha)\cdot 2}\right)+\sqrt{\frac{1}{4}\cdot\left(\frac{\lambda\cdot\sqrt{f\cdot f'}}{d(f,\alpha)\cdot 2}\right)^2+\delta\cdot f\cdot f'}\,.$$

f is the separation between source focus and the observed mirror segment, f' is the separation between the observed mirror segment and image focus. Due to the high eccentricity ($a>>b,c$) of the reflectors observed herein, $f\approx x$ and $f'\approx 2a-x$. δ is the dispersion coefficient of the multiple layers used (see e.g. US 6,226,349).

If the irregularity of the coating as described above can be described e.g. by $d(f,\alpha)=d_0(f)\cdot\cos\beta$ with $\beta=\arctan\frac{dz}{dy}$. The angular dependence of the elliptic semi-axis *b* can be described by

$$b(\beta)=\frac{1}{2}\cdot\left(\frac{\lambda\cdot\sqrt{f\cdot f'}}{d_0(f)\cdot\cos\beta\cdot 2}\right)+\sqrt{\frac{1}{4}\cdot\left(\frac{\lambda\cdot\sqrt{f\cdot f'}}{d_0(f)\cdot\cos\beta\cdot 2}\right)^2+\delta\cdot f\cdot f'}$$

The ellipsoidal equation then becomes

$$\frac{(x-a)^2}{a^2}+\frac{r^2}{\left(\frac{1}{2}\cdot\left(\frac{\lambda\cdot\sqrt{f\cdot f'}}{d_0(f)\cdot\cos\beta\cdot 2}\right)+\sqrt{\frac{1}{4}\cdot\left(\frac{\lambda\cdot\sqrt{f\cdot f'}}{d_0(f)\cdot\cos\beta\cdot 2}\right)^2+\delta\cdot f\cdot f'}\right)^2}=1\,.$$

For the further analysis $1-\frac{(x-a)^2}{a^2}=\frac{r_0^2}{b_0^2}$ can be defined, which leads to the following equation

$$r_0 \cdot \left(\frac{1}{2} \cdot \left(\frac{\lambda \cdot \sqrt{f \cdot f'}}{d_0(f) \cdot \cos\beta \cdot 2} \right) + \sqrt{\frac{1}{4} \cdot \left(\frac{\lambda \cdot \sqrt{f \cdot f'}}{d_0(f) \cdot \cos\beta \cdot 2} \right)^2 + \delta \cdot f \cdot f'} \right) = r \cdot b_0$$

which, solved for $\cos\beta$, gives

$$\cos\beta = \frac{1}{d_0(f)} \cdot \frac{\lambda \cdot r \cdot b_0 \cdot r_0 \cdot \sqrt{f \cdot f'}}{2 \cdot \left(r^2 \cdot b_0^2 - \delta \cdot f \cdot f' \cdot r_0^2\right)}$$

To determine the cross-sectional shape $z = f(y)$ a numerical solution is recommended – with the initial conditions $\beta(0) = 0$ and $z(0) = -r_0$. The algorithm is

$$\left(\frac{dz}{dy}\right)_i = \tan\beta_i$$

$$z_{i+1} = z_i + \left(\frac{dz}{dy}\right)_i \cdot \Delta y$$

$$y_{i+1} = y_i + \Delta y$$

$$\cos\beta_{i+1} = \frac{1}{d_0(f)} \cdot \frac{\lambda \cdot \sqrt{y_{i+1}^2 + z_{i+1}^2} \cdot b_0 \cdot r_0 \cdot \sqrt{f \cdot f'}}{2 \cdot \left(\left(y_{i+1}^2 + z_{i+1}^2\right) b_0^2 - \delta \cdot f \cdot f' \cdot r_0^2\right)}$$

Refined numerical solutions according to known methods are possible. Ray tracing simulations however show that this solution is sufficiently accurate.

The calculated cross-sectional shape is shown in Fig. 16. In contrast to the rotationally symmetrical shape (b=c=5mm), the shape described herein is flatter and corresponds with good approximation to an ellipsoid with b=6.4mm and c=5mm. Ray tracing calculations confirm that an ellipsoid modified in this manner reflects the desired

X-ray line over the entire cross-section, despite the coating error. In contrast to Fig. 14b, the desired monochromatic effect is also completely maintained. The flatter shape of the inventive solution has moreover only approximately half the edge inclination than the rotationally symmetrical ellipsoid. For this reason, one can expect that the coating problems and the production problems of the curved shape be additionally substantially reduced by the low roughness requirements. Production of the inventive reflectors is therefore simpler and less expensive.

Analog to the above-described method, a non-rotationally symmetrical paraboloid can be calculated to parallelize rather than focus the beam. The rotation paraboloid with the parabolic parameter p is preferably expressed in cylindrical coordinates:

$$r^2 = 2 \cdot p \cdot x$$

wherein $z = r \cdot \cos\alpha$ and $y = r \cdot \sin\alpha$.

To ensure optimum reflection of a rotationally paraboloid mirror, the following must be true for the coating thickness d :

$$d(\alpha) = const.$$

A coating error can be corrected through variation of p with α. The paraboloid of rotation then becomes the generally non-rotationally symmetrical paraboloid.

$$r^2 = 2 \cdot p(\alpha) \cdot x .$$

$p(\alpha)$ is calculated according to

$$d(f,\alpha)=\frac{\lambda\cdot\sqrt{2\cdot p(\alpha)\cdot f}}{2\cdot(p(\alpha)-2\cdot\delta\cdot f)}$$

[publication Schuster see above]. One obtains

$$\sqrt{p(\alpha)}=\frac{1}{2}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d(f,\alpha)\cdot 2}\right)+\sqrt{\frac{1}{4}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d(f,\alpha)\cdot 2}\right)^2+2\cdot\delta\cdot f}\,.$$

If the irregularity of the coating can again be described as $d(f,\alpha)=d_0(f)\cdot\cos\beta$, wherein $\beta=\arctan\frac{dz}{dy}$, the angular dependence of the parabolic parameter p is given by

$$\sqrt{p(\beta)}=\frac{1}{2}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d_0(f)\cdot\cos\beta\cdot 2}\right)+\sqrt{\frac{1}{4}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d_0(f)\cdot\cos\beta\cdot 2}\right)^2+2\cdot\delta\cdot f}$$

The paraboloid equation then becomes

$$r^2=2\cdot\left(\frac{1}{2}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d_0(f)\cdot\cos\beta\cdot 2}\right)+\sqrt{\frac{1}{4}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d_0(f)\cdot\cos\beta\cdot 2}\right)^2+2\cdot\delta\cdot f}\right)^2\cdot x$$

For further analysis $x=\frac{r_0^{\,2}(x)}{2\cdot p_0}$ can be defined. The result is

$$r_0\cdot\left(\frac{1}{2}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d_0(f)\cdot\cos\beta\cdot 2}\right)+\sqrt{\frac{1}{4}\cdot\left(\frac{\lambda\cdot\sqrt{2\cdot f}}{d_0(f)\cdot\cos\beta\cdot 2}\right)^2+2\cdot\delta\cdot f}\right)=r\cdot p_0\,,$$

which, solved for $\cos\beta$, becomes

$$\cos\beta = \frac{1}{d_0(f)} \cdot \frac{\lambda \cdot \sqrt{2 \cdot r \cdot p_0 \cdot r_0 \cdot f}}{2 \cdot (r \cdot p_0 - 2 \cdot \delta \cdot f \cdot r_0)}$$

To determine the cross-sectional shape $z = f(y)$ a numerical solution is recommended – with the initial conditions $\beta(0) = 0$ and $z(0) = -r_0$.

The algorithm is:

$$\left(\frac{dz}{dy}\right)_i = \tan\beta_i$$

$$z_{i+1} = z_i + \left(\frac{dz}{dy}\right)_i \cdot \Delta y$$

$$y_{i+1} = y_i + \Delta y$$

$$\cos\beta_{i+1} = \frac{1}{d_0(f)} \cdot \frac{\lambda \cdot \sqrt{2 \cdot \sqrt{{y_{i+1}}^2 + {z_{i+1}}^2} \cdot p_0 \cdot r_0 \cdot f}}{2 \cdot \left(\sqrt{{y_{i+1}}^2 + {z_{i+1}}^2} \cdot p_0 - 2 \cdot \delta \cdot f \cdot r_0\right)}$$

Refined numerical solutions according to conventional methods are possible. Ray tracing simulations, however, show that the solution shown herein provides sufficient accuracy.

The two approaches described above are to be understood as examples only and analog approaches are possible for other coating errors (e.g. parabolic, $(\cos\beta)^n$) and other reflector shapes (e.g. spherical, hyperboloid, ...).

The curved reflector substrates can be produced in a manner known per se e.g. by grinding, polishing, and lapping of solid bodies of quartz, Zerodur, glass or other materials. Roughnesses below 0.1nm (already 0.3nm is satisfactory for multi-layers) and curvature errors below 5µrad (already less than 25µrad produces very good mirrors) were routinely obtained for reflectors according to US 6,226,349 using such methods. These values lead to exceptional optical properties. Further shaping techniques of the reflector substrates are bending technologies [e.g.. DE 19935513] or copying/replication techniques [US 4,525,853 claim 12].

The advantages of the inventive teaching can be summarized as follows:

a) the production of the shape is facilitated since flatter shapes with less curvatures and edge angles can be used. The flatter shape facilitates polishing to reduce roughness.

b) Selection of the cross-sectional shape permits further favorable influence on the radiation properties (beam size, divergence), e.g. to produce a wider beam depending on the application. To determine mechanical tensions or textures of materials with X-ray diffractometric methods, it is desired to illuminate a larger sample surface (in contrast to monocrystal diffractometry). Selection of a non-rotationally symmetrical reflector provides a larger selection of optics optimized for the application. The optical design permits more flexibility.

c) Especially for multi-layer X-ray mirrors the following is also true:

Coating errors in a transverse direction can be completely compensated for through (free!) selection of the cross-sectional shape of the body in this direction. The coating becomes then "very" simple" or becomes possible for the first time with the same techniques which are currently used for substantially flat optics.

d) Intensity is considerably increased since, in contrast to prior art, only one reflection is required (intensity loss per reflection approximately 50%) and since a larger mirror surface can be used. Conventional reflectors are used within a width of only approximately 1mm. In contrast thereto, a 4mm wide reflector was described (without limitation of the general case). In total, an intensity gain by a factor of 8 can be expected.

e) Only one mirror is required instead of the optics according to prior art having 2 mirrors (cost factor).

f) Adjustment of the reflector is much easier than for a Kirkpatrick-Baez arrangement according to prior art.

Due to the particularly advantageous embodiment of the inventive reflector as a Goebel mirror with a non-rotationally symmetrical curvature transverse to the x direction (which corresponds approximately to the main irradiation direction of the X-ray radiation) the design of such an embodiment or of an associated X-ray analysis device is explained in more detail below.

The preferred inventive X-ray analysis device comprises

- a source emitting X-ray radiation
- a sample to be analyzed

- a detector which responds to X-ray radiation
- optical shaping and/or delimiting means; and
- a curved multi-layer Bragg reflector which is disposed in the optical path between the source and the sample and comprises a periodically repeating sequence of layers, wherein one period consists of at least two individual layers A, B which have different diffraction index decrements $\delta_A \neq \delta_B$ and thicknesses d_A and d_B,
- wherein the period thickness, i.e. the sum $d = d_A + d_B + \ldots$ of the individual layers A, B, ... of a period changes continuously along an x-direction, and
- wherein the reflector is curved such that it forms a partial surface of a paraboloid or ellipsoid in the focal line or focal point at which the source or an image of the source is located,
- wherein the paraboloid or ellipsoid is curved along a cross-section in a plane perpendicular to the x-direction in a shape which is not that of a circular arc. The paraboloid or ellipsoid is not a rotational paraboloid or ellipsoid, rather a non-rotationally symmetrical paraboloid or ellipsoid.

The embodiments of the inventive X-ray analysis device with parabolic reflector shape have the following properties:

- the layers of the reflector are vacuum-evaporated, sputtered or grown directly on a concavely curved surface of a parabolic hollowed substrate, wherein the curvature of the concave substrate surface in a xz plane follows the formula $z^2 = 2px$ with 0,02 mm < p < 0,5 mm, preferably $p \approx 0{,}1$ mm;
- the concave substrate surface facing the reflector has a maximum admissible shape deviation of $\Delta p = \sqrt{2px} \cdot \Delta\Theta_R$, wherein $\Delta\Theta_R$ is the half-width of the Bragg reflection of the

reflector and is in the range $0{,}01° < \Delta\Theta_R < 0{,}5°$, preferably $0{,}02° < \Delta\Theta_R < 0{,}20°$,

- the concave substrate surface facing the reflector has a maximum admissible waviness of $\frac{\Delta z}{\Delta x} = \frac{1}{2}\Delta\Theta_R$,
- the concave substrate surface facing the reflector has a maximum admissible roughness of $\Delta z = \frac{d}{2\pi}$, preferably $\Delta z \leq 0{,}3$ nm,
- the X-ray radiation impinges on the curved surface of the reflector at an angle of incidence of $0° \leq \Theta \leq 5°$,
- the periodic thickness d along the x-direction changes such that the X-ray radiation of a certain wavelength λ of a point X-ray source always experiences a Bragg reflection irrespective of the point of incidence (x, z) on the reflector in that the periodic thickness d increases in x-direction towards the paraboloid opening according to $d = \frac{\lambda}{2} \frac{1}{(1-\bar{\delta}/\sin^2\Theta)\sin\Theta}$ and $\Theta = \operatorname{arc\,cot}\frac{\sqrt{2px}}{p}$, wherein $\bar{\delta}$ is the decrease of the average refractive index of the multi-layer Bragg reflector,
- the deviation $\Delta d/\Delta x$ of the periodic thickness d at each point of the multi-layer Bragg reflector along the x direction is smaller than $\frac{\Delta d}{\Delta x} = \frac{1}{2}\frac{d}{x}$,
- the following is true for the periodic thickness d: $1 \text{ nm} \leq d \leq 20$ nm,
- for the number N of periods $10 < N < 500$, preferably $50 \leq N \leq 100$,

- and the energy E of the light quantum of the X-ray radiation is: 0,1 keV < E < 0,1 MeV.

Use of amorphous or polycrystalline substrate material is also advantageous, in particular glass, amorphous Si, polycrystalline ceramic material or plastic material. With regard to the number of individual layers per period, 2, 3 or 4 layers are particularly recommended. The layer thicknesses of the individual layers differ from material to material, preferably by at most 5%.

Conventional (rotationally symmetrical) Goebel mirrors according to prior art are described e.g. in DE 198 33 524 A1 the entire disclosure of which is hereby incorporated by reference.